

Toluene
108-88-3 | DTXSID7021360

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 3.87

Global applicability domain: Inside

Local applicability domain index: 9.93e-01

Confidence level: 5.64e-01

Nearest Neighbors from the Training Set

Image not found

Toluene

Measured: 3.31

Predicted: 3.87

Image not found

Hexanal

Measured: 4.41

Predicted: 3.86

Image not found

Methylcyclohexane

Measured: 3.03

Predicted: 3.59

Image not found

2-Hexanone

Measured: 3.68

Predicted: 3.66

Image not found

Dimethyl sulfoxide

Measured: 4.96

Predicted: 3.99